



**Inchi:** Tardigal  
 Tri-digitoxoside  
 Unidigin  
**InchiKey:** InChI=1S/C41H64O13/c1-20-36(46)29(42)16-34(49-20)53-38-22(3)51-35(18-31(38)44)5  
**InchiKey:** WDJUZGPOPHTGOT-UCKSZOHFSA-N  
**Formula:** C41H64O13  
**SMILES:** CC1OC(OC2C(O)CC(OC3C(O)CC(OC4CCC5(C)C(CCC6C5CCC5(C)C(C7=CC(=O)OC7  
**Mol. weight [g/mol]:** 764.94  
**CAS:** 71-63-6

## Physical Properties

Property code	Value	Unit	Source
gf	-968.09	kJ/mol	Joback Method
hf	-2381.29	kJ/mol	Joback Method
hfus	103.65	kJ/mol	Joback Method
hvap	215.62	kJ/mol	Joback Method
log10ws	-5.28		Aqueous Solubility Prediction Method
log10ws	-5.29		Estimated Solubility Method
logp	3.247		Crippen Method
mcvol	569.380	ml/mol	McGowan Method
pc	795.28	kPa	Joback Method
tb	1912.32	K	Joback Method
tc	3108.43	K	Joback Method
tf	528.65	K	Aqueous Solubility Prediction Method
vc	2.067	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	3852.19	J/molxK	1912.32	Joback Method
cpg	4580.17	J/molxK	2111.67	Joback Method
cpg	5558.09	J/molxK	2311.02	Joback Method
cpg	6836.53	J/molxK	2510.37	Joback Method
cpg	8466.10	J/molxK	2709.72	Joback Method
cpg	10497.39	J/molxK	2909.08	Joback Method

## Sources

<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>Aqueous Solubility Prediction Method:</b>	<a href="http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa">http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa</a>
<b>Estimated Solubility Method:</b>	<a href="http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt">http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C71636&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C71636&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvac:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mccvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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